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The photodecomposition product μ-oxalato-1κ^2O,O':2κ^2O'',O'''-bis{bis[2-(2-pyridyl)phenyl-κ^2C,N]iridium(III)}–acetone (1/1.974)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
Disorder in solvent or counterion
R factor = 0.040
wR factor = 0.098
Data-to-parameter ratio = 21.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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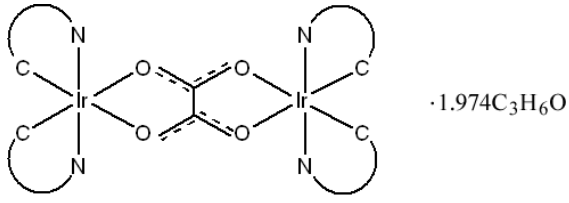
An attempt to grow crystals of [Ir(ppy)$_2$(vacac)], (I), from an acetone-d_6 solution formed instead crystals of [{Ir(ppy)$_2$}$_2$(μ-oxalato)] acetone solvate, (II), [Ir$_2$(C$_{11}$H$_8$N)$_4$(C$_2$O$_4$)]·1.974C$_3$H$_6$O, where ppy is the phenylpyridine anion and vacac is vinylacetylacetonate. Each Ir^{III} ion in (II) is in a pseudo-octahedral coordination environment, where the pyridine N atoms are *trans* to each other and the phenyl C atoms are *trans* to the O atoms of the oxalate bridging ligand. There are two crystallographically independent dimer molecules, each lying on an inversion centre. It is suggested that the oxalate ligand is formed in a series of steps initiated by the aldol condensation of acetone with vacac.

Comment

The excited state of cyclometallated iridium(III) complexes is readily quenched by oxygen and this makes these complexes ideal for incorporation into oxygen-sensing devices. We recently published a study demonstrating their utility (DeRosa *et al.*, 2003), as well as a study describing the syntheses of a number of promising iridium complexes (DeRosa *et al.*, 2004).



(II)

In an attempt to grow crystals of [Ir(ppy)$_2$(vacac)], (I), where ppy is the phenylpyridine anion and vacac is vinyl acetylacetonate, from an acetone-d_6 solution of the complex, golden-yellow crystals of the dimer [{Ir(ppy)$_2$}$_2$(μ-oxalato)] acetone solvate (1/1.974), (II), were isolated. We present here the crystal structure of (II).

Crystallography revealed the space group of (II) to be triclinic, $P\overline{1}$, with both Ir dimers of the unit cell centred on inversion centres, and the presence of acetone in the crystal structure. The asymmetric unit consists of two half-dimers (both being completed across an inversion centre), one fully occupied ordered acetone site, one partially occupied acetone

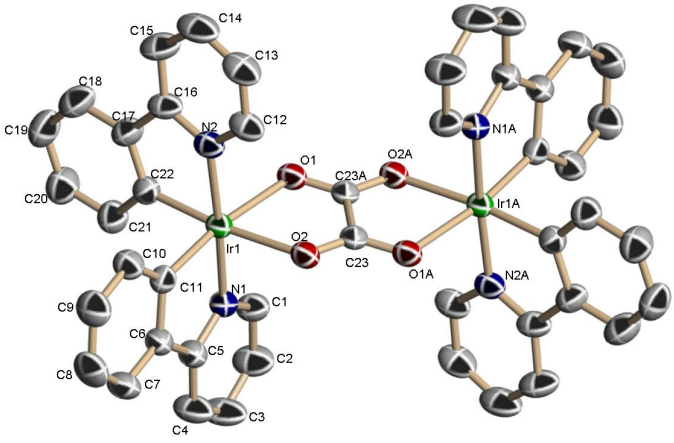


Figure 1
The molecular structure of (II). All acetone molecules and H atoms have been omitted for clarity. Only one of the two crystallographically independent molecules is depicted. Anisotropic displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: A, $1-x$, $-y$, $1-z$.]

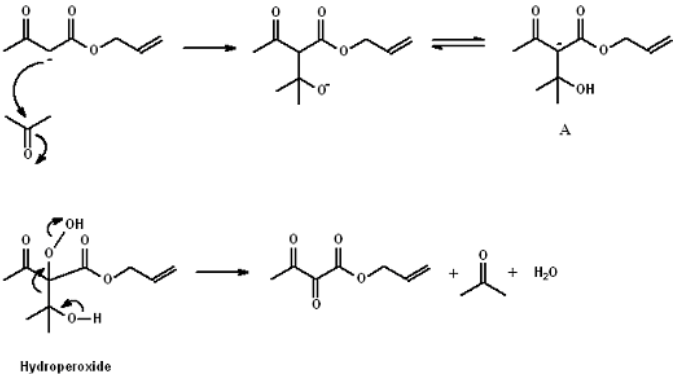


Figure 2
Aldol condensation between the vacac ligand and acetone, and the dehydration of the hydroperoxide that is formed from *A* reacting with singlet oxygen.

site [occupancy 0.234 (3)], and one partially occupied and disordered (overlapped) acetone site [occupancies of 0.531 (3) and 0.209 (3)]. The asymmetric unit thus contains the equivalent of one Ir dimer cluster and 1.974 acetone molecules.

Each Ir^{III} ion in (II) is in a pseudo-octahedral coordination environment, where the pyridine N atoms are *trans* to each other and the phenyl C atoms are *trans* to the O atoms of the oxalate bridging ligand. Fig. 1 shows the molecular structure of one of the iridium dimers, and selected structural data are compiled in Table 1.

The formation of complex (II) from (I) is unexpected. Oxalate was not added to the reaction mixture, nor is oxalate associated with the synthesis of (I). Complex (II) did not form in $CHCl_3$, CH_3CN or methanol, or if under an argon atmosphere, or if shielded from light. Because acetone is required for the formation of (II), it is suggested that the initial step involves an aldol condensation between the enolate vacac

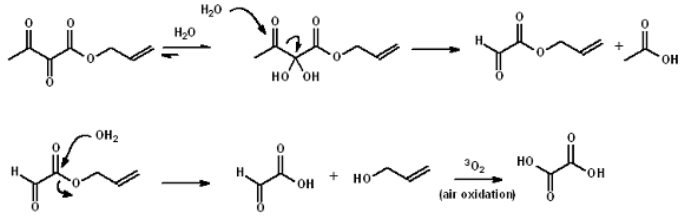


Figure 3
Cleavage of the tricarbonyl and formation of oxalic acid.

anion and acetone (Fig. 2) (Wasserman & Ives, 1981; Wasserman, 2004).

Dioxygen quenching of the excited state of (I) likely produces singlet oxygen which attacks the aldol condensation product *A* (Fig. 2), forming a hydroperoxide which can then dehydrate to form the tricarbonyl species. The tricarbonyl species can be easily hydrated to the geminal-diol and further hydrolysis can form the aldehydo ester (Rubin & Gleiter, 2000). Hydrolysis of the allyl ester and air oxidation of the aldehyde gives oxalic acid (Fig. 3).

The formation of (II) is indicative that $[Ir(ppy)_2(vacac)]$ is subject to decomposition and this may have implications in its use in oxygen-sensor applications.

Experimental

$[Ir(ppy)_2(vacac)]$ (10 mg) was dissolved in acetone-d_6 (1 ml) and placed in an NMR tube. No attempt was made to exclude air from the tube. The tube was left sealed, but unshielded from light, for four weeks. Small golden crystals of (II) were harvested from the NMR tube for X-ray crystallography. IR: ν(C═O) 1617 cm^{-1}. The complex could also be prepared by reacting oxalate with (μ-dichloro)tetrakis(phenylpyridine)diiridium(III).

Crystal data

$[Ir(C_{11}H_8N)_4(C_2O_4)]\cdot 1.974C_3H_6O$
M_r = 1203.79
Triclinic, $P\overline{1}$
a = 9.9708 (5) Å
b = 13.0403 (7) Å
c = 19.3556 (10) Å
α = 103.383 (1)°
β = 99.003 (1)°
γ = 98.203 (1)°
V = 2375.9 (2) $Å^3$
Z = 2
D_x = 1.683 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8192 reflections
θ = 1.7–29.6°
μ = 5.65 mm^{-1}
T = 173 (2) K
Block, gold
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.430, T_{max} = 0.568
30 150 measured reflections
13 184 independent reflections
9639 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 29.6°
$h = -13 \rightarrow 13$
$k = -18 \rightarrow 18$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.098
S = 1.01
13184 reflections
602 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.9043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.040
$\Delta\rho_{max}$ = 2.37 e $Å^{-3}$
$\Delta\rho_{min}$ = −1.13 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Ir1—C22	1.979 (2)	Ir1′—C11′	1.9876 (19)
Ir1—C11	1.9824 (19)	Ir1′—N1′	2.0191 (17)
Ir1—N1	2.0308 (13)	Ir1′—N2′	2.0303 (18)
Ir1—N2	2.0429 (14)	Ir1′—O1′	2.1931 (13)
Ir1—O2	2.1911 (14)	Ir1′—O2′	2.1969 (15)
Ir1—O1	2.1938 (13)	O1—C23^{i}	1.238 (2)
Ir1′—C22′	1.980 (2)		
N1—Ir1—N2	175.79 (7)	C22′—Ir1′—C11′	89.48 (8)
N2—Ir1—O2	96.11 (6)	C22′—Ir1′—N1′	96.51 (8)
C22—Ir1—O1	98.03 (7)	C11′—Ir1′—N1′	80.88 (8)
C11—Ir1—O1	171.29 (7)	C22′—Ir1′—N2′	80.65 (8)
N1—Ir1—O1	94.75 (5)	C11′—Ir1′—N2′	94.79 (8)
N2—Ir1—O1	85.70 (5)	N1′—Ir1′—N2′	174.88 (7)
O2—Ir1—O1	76.18 (5)		

Symmetry code: (i) $-x+1, -y, -z+1$.

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–0.98 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl atoms. First- and second-neighbour distance restraints were applied to the disordered solvent molecules. Equal anisotropic displacement parameter restraints were applied to three pairs of disordered atoms of solvent molecules that almost overlap. The highest peak and the deepest hole in the final Fourier map are 0.80 and 1.36 Å, respectively, from the Ir atom.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial support from the Natural Science and Engineering Research Council of Canada, in the form of a Discovery Grant (RJC) and a postgraduate scholarship (MCD), is gratefully acknowledged. CEBE thanks the NRC for supporting his research through the Research Associate Program.

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supporting information

Acta Cryst. (2005). E**61**, m967–m969 [doi:10.1107/S1600536805008809]

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Crystallography revealed the space group of (II) to be triclinic, $P\overline{1}$, with both Ir dimers of the unit cell centred on inversion centres, and the presence of acetone in the crystal lattice. The asymmetric unit consists of two half-dimers (both being completed across the inversion centre), one fully occupied ordered acetone site, one partially occupied acetone site (occupancy 0.234), and one partially occupied and disordered (overlapped) acetone site (occupancies of 0.531 and 0.209). The asymmetric unit thus contains the equivalent of one Ir dimer cluster and 1.974 acetone molecules.

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Dioxygen quenching of the excited state of (I) likely produces singlet oxygen which attacks the aldol condensation product *A* (Fig. 2), forming a hydroperoxide which can then dehydrate to form the tricarbonyl species. The tricarbonyl species can be easily hydrated to the geminal-diol and further hydrolysis can form the aldehydo ester (Rubin & Gleiter, 2000). Hydrolysis of the allyl ester and air oxidation of the aldehyde gives the oxalate molecule (Fig. 3).

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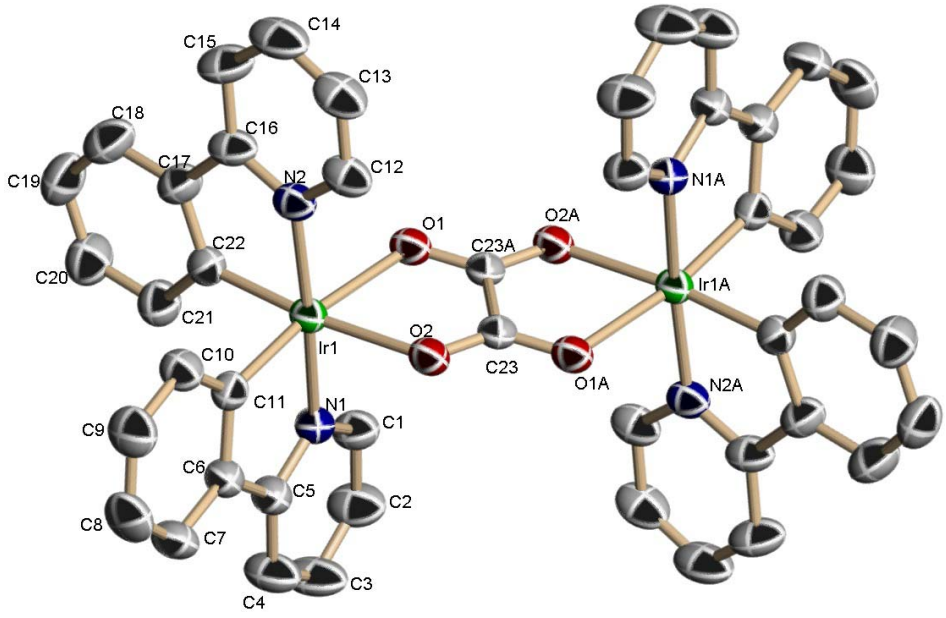
prepared by reacting oxalate with (μ-dichloro)tetrakis(phenylpyridine)diiridium(III).

S3. Refinement

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for methyl atoms. **Please check added text.** First- and second-neighbour distance restraints using the *DFIX* instruction in *SHELXL* (Sheldrick, 1997) were applied to the disordered solvent molecules. Equal anisotropic displacement parameter restraints (EADP instruction) were applied to three pairs of disordered atoms of solvent molecules that almost overlap. The highest peak and the deepest hole in the final Fourier map are 0.80 and 1.36 Å, respectively, from the Ir atom.



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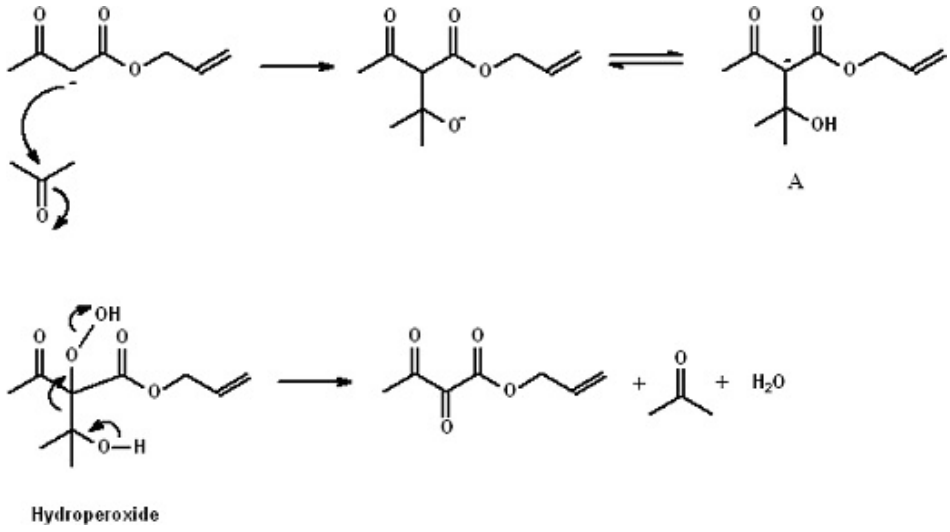

Figure 2

Aldol condensation between the vacac ligand and acetone, and the dehydration of the hydroperoxide that is formed from *A* reacting with singlet oxygen.

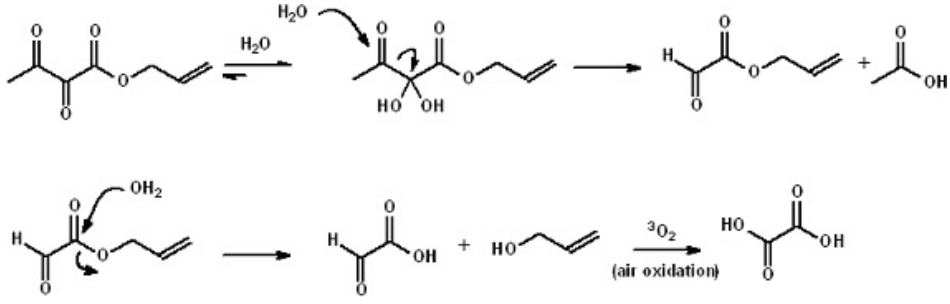

Figure 3

Cleavage of the tricarbonyl and formation of the oxalate ligand.

μ-oxalato-1κ^2O,O':2κ^2O'',O'''tetrakis(phenylpyridine-κ^2C,N)\- diiridium(III) acetone 1.974 solvate

Crystal data

$[Ir(C_2O_4)(C_{11}H_8N)_4]\cdot 1.974C_3H_6O$
$M_r = 1203.79$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.9708$ (5) Å
$b = 13.0403$ (7) Å
$c = 19.3556$ (10) Å
$\alpha = 103.383$ (1)°
$\beta = 99.003$ (1)°
$\gamma = 98.203$ (1)°
$V = 2375.9$ (2) Å^3
$Z = 2$
$F(000) = 1170$
$D_x = 1.683$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8192 reflections
$\theta = 1.7$–29.6°
$\mu = 5.65$ mm^{-1}
$T = 173$ K
Block, gold
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.430, T_{max} = 0.568
30150 measured reflections
13184 independent reflections
9639 reflections with $I > 2\sigma(I)$

R_{int} = 0.044
θ_{max} = 29.6°, θ_{min} = 1.7°
h = −13→13
k = −18→18
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.098
S = 1.01
13184 reflections
602 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.9043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.040
$\Delta\rho_{max}$ = 2.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ir1	0.333434 (7)	0.133535 (5)	0.446300 (4)	0.02833 (2)	
Ir1′	0.362785 (7)	0.627249 (6)	0.095088 (4)	0.03433 (2)	
O1	0.51118 (12)	0.05688 (10)	0.42742 (7)	0.0325 (3)	
O2	0.37124 (12)	0.05975 (10)	0.53663 (7)	0.0329 (4)	
O1′	0.34793 (13)	0.46263 (11)	0.03022 (7)	0.0375 (4)	
O2′	0.54098 (14)	0.63805 (11)	0.04149 (7)	0.0397 (4)	
N1	0.18998 (15)	0.00040 (12)	0.39304 (8)	0.0331 (4)	
N2	0.47597 (15)	0.27106 (12)	0.49302 (9)	0.0340 (4)	
N1′	0.49092 (16)	0.60726 (14)	0.18067 (9)	0.0399 (5)	
N2′	0.22824 (18)	0.65759 (13)	0.01539 (9)	0.0421 (5)	
C1	0.2177 (2)	−0.08684 (16)	0.34887 (11)	0.0400 (6)	
H1	0.3102	−0.0881	0.3428	0.048*	
C2	0.1173 (2)	−0.17347 (18)	0.31264 (14)	0.0551 (8)	
H2	0.1391	−0.2338	0.2813	0.066*	
C3	−0.0151 (2)	−0.1718 (2)	0.32232 (15)	0.0611 (8)	
H3	−0.0863	−0.2318	0.2982	0.073*	
C4	−0.0458 (2)	−0.08301 (18)	0.36708 (14)	0.0526 (7)	
H4	−0.1379	−0.0819	0.3739	0.063*	
C5	0.05789 (19)	0.00445 (15)	0.40197 (11)	0.0363 (5)	

C6	0.04163 (19)	0.10710 (15)	0.44648 (11)	0.0349 (5)
C7	−0.0838 (2)	0.13056 (18)	0.46267 (12)	0.0453 (6)
H7	−0.1647	0.0765	0.4465	0.054*
C8	−0.0914 (2)	0.23063 (19)	0.50161 (13)	0.0531 (7)
H8	−0.1772	0.2464	0.5122	0.064*
C9	0.0276 (2)	0.30909 (18)	0.52551 (13)	0.0521 (7)
H9	0.0225	0.3787	0.5525	0.062*
C10	0.1528 (2)	0.28741 (16)	0.51061 (11)	0.0383 (6)
H10	0.2326	0.3424	0.5276	0.046*
C11	0.16490 (18)	0.18546 (14)	0.47069 (10)	0.0309 (5)
C12	0.55132 (19)	0.29571 (17)	0.56057 (11)	0.0401 (6)
H12	0.5320	0.2502	0.5911	0.048*
C13	0.6552 (2)	0.38425 (18)	0.58715 (13)	0.0491 (7)
H13	0.7049	0.4008	0.6356	0.059*
C14	0.6861 (2)	0.44829 (19)	0.54261 (15)	0.0576 (8)
H14	0.7586	0.5092	0.5594	0.069*
C15	0.6101 (2)	0.42279 (18)	0.47308 (14)	0.0520 (7)
H15	0.6314	0.4658	0.4414	0.062*
C16	0.5021 (2)	0.33424 (15)	0.44888 (11)	0.0380 (6)
C17	0.4120 (2)	0.29878 (15)	0.37732 (11)	0.0386 (5)
C18	0.4151 (3)	0.35527 (18)	0.32429 (13)	0.0527 (7)
H18	0.4777	0.4214	0.3342	0.063*
C19	0.3283 (3)	0.31591 (18)	0.25800 (13)	0.0538 (7)
H19	0.3291	0.3553	0.2224	0.065*
C20	0.2397 (3)	0.21851 (18)	0.24332 (13)	0.0522 (7)
H20	0.1816	0.1900	0.1969	0.063*
C21	0.2348 (2)	0.16169 (17)	0.29592 (11)	0.0433 (6)
H21	0.1719	0.0956	0.2852	0.052*
C22	0.32132 (18)	0.20062 (14)	0.36423 (10)	0.0327 (5)
C23	0.46067 (17)	0.00014 (14)	0.53137 (9)	0.0286 (5)
C1′	0.5299 (2)	0.51368 (18)	0.18534 (11)	0.0447 (6)
H1′	0.4928	0.4514	0.1467	0.054*
C2′	0.6216 (2)	0.5048 (2)	0.24422 (12)	0.0498 (7)
H2′	0.6479	0.4381	0.2459	0.060*
C3′	0.6733 (2)	0.5945 (2)	0.29992 (12)	0.0523 (7)
H3′	0.7367	0.5904	0.3409	0.063*
C4′	0.6340 (2)	0.69079 (19)	0.29705 (12)	0.0457 (6)
H4′	0.6691	0.7526	0.3363	0.055*
C5′	0.54292 (19)	0.69752 (18)	0.23668 (11)	0.0414 (6)
C6′	0.4934 (2)	0.79181 (17)	0.22350 (11)	0.0404 (6)
C7′	0.5351 (2)	0.89533 (19)	0.27230 (12)	0.0504 (7)
H7′	0.5974	0.9052	0.3168	0.060*
C8′	0.4855 (3)	0.98123 (19)	0.25546 (13)	0.0562 (8)
H8′	0.5125	1.0504	0.2884	0.067*
C9′	0.3980 (3)	0.9669 (2)	0.19161 (14)	0.0609 (8)
H9′	0.3645	1.0270	0.1804	0.073*
C10′	0.3549 (2)	0.86603 (18)	0.14134 (13)	0.0498 (7)
H10′	0.2929	0.8584	0.0971	0.060*

C11′	0.4039 (2)	0.77698 (16)	0.15697 (11)	0.0390 (6)	
C12′	0.2659 (3)	0.69184 (19)	−0.04096 (13)	0.0574 (8)	
H12′	0.3603	0.7006	−0.0452	0.069*	
C13′	0.1701 (3)	0.7143 (2)	−0.09224 (15)	0.0719 (10)	
H13′	0.1973	0.7384	−0.1316	0.086*	
C14′	0.0341 (3)	0.7008 (2)	−0.08495 (16)	0.0737 (10)	
H14′	−0.0336	0.7155	−0.1198	0.088*	
C15′	−0.0043 (3)	0.6672 (2)	−0.02925 (15)	0.0643 (9)	
H15′	−0.0989	0.6571	−0.0254	0.077*	
C16′	0.0945 (2)	0.64706 (17)	0.02308 (13)	0.0491 (7)	
C17′	0.0713 (2)	0.61467 (18)	0.08750 (13)	0.0485 (7)	
C18′	−0.0598 (2)	0.5979 (2)	0.10718 (15)	0.0626 (9)	
H18′	−0.1393	0.6079	0.0773	0.075*	
C19′	−0.0714 (2)	0.5674 (2)	0.16910 (15)	0.0666 (9)	
H19′	−0.1591	0.5577	0.1825	0.080*	
C20′	0.0423 (2)	0.5505 (2)	0.21236 (13)	0.0599 (8)	
H20′	0.0320	0.5266	0.2544	0.072*	
C21′	0.1729 (2)	0.56836 (19)	0.19464 (12)	0.0509 (7)	
H21′	0.2511	0.5581	0.2255	0.061*	
C22′	0.1901 (2)	0.60126 (16)	0.13201 (11)	0.0400 (6)	
C23′	0.55548 (18)	0.54999 (15)	0.00349 (10)	0.0328 (5)	
O101	0.8231 (3)	0.42152 (18)	0.35311 (15)	0.1089 (10)	
C101	0.9857 (3)	0.3143 (3)	0.3262 (2)	0.1011 (14)	
H10A	1.0502	0.3831	0.3424	0.152*	
H10B	0.9886	0.2799	0.2758	0.152*	
H10C	1.0121	0.2677	0.3570	0.152*	
C102	0.8491 (3)	0.3319 (2)	0.33088 (17)	0.0722 (10)	
C103	0.7381 (4)	0.2374 (3)	0.3079 (2)	0.0985 (15)	
H10D	0.6495	0.2598	0.3125	0.148*	
H10E	0.7554	0.1886	0.3385	0.148*	
H10F	0.7352	0.2006	0.2573	0.148*	
C01A	0.8697 (4)	0.9800 (3)	0.1364 (4)	0.0963 (19)	0.209 (3)
C02A	0.9601 (5)	0.8988 (4)	0.1349 (9)	0.151 (3)	0.209 (3)
H02A	1.0570	0.9351	0.1500	0.227*	0.209 (3)
H02B	0.9450	0.8524	0.0856	0.227*	0.209 (3)
H02C	0.9378	0.8553	0.1681	0.227*	0.209 (3)
C03A	0.7407 (5)	0.9498 (9)	0.0808 (4)	0.151 (3)	0.209 (3)
H03A	0.6884	1.0083	0.0873	0.227*	0.209 (3)
H03B	0.6848	0.8847	0.0858	0.227*	0.209 (3)
H03C	0.7636	0.9364	0.0325	0.227*	0.209 (3)
O01A	0.9169 (10)	1.0734 (3)	0.1688 (6)	0.132 (2)	0.209 (3)
C01B	0.8867 (3)	0.9744 (2)	0.1379 (3)	0.0963 (19)	0.531 (3)
C02B	1.0089 (4)	0.9277 (4)	0.1224 (5)	0.151 (3)	0.531 (3)
H02D	1.0727	0.9790	0.1076	0.227*	0.531 (3)
H02E	0.9794	0.8614	0.0834	0.227*	0.531 (3)
H02F	1.0555	0.9117	0.1661	0.227*	0.531 (3)
C03B	0.7675 (4)	0.8970 (4)	0.1427 (4)	0.151 (3)	0.531 (3)
H03D	0.6953	0.9356	0.1581	0.227*	0.531 (3)

H03E	0.7969	0.8577	0.1781	0.227*	0.531 (3)
H03F	0.7311	0.8463	0.0952	0.227*	0.531 (3)
O01B	0.8909 (5)	1.0701 (2)	0.1533 (3)	0.132 (2)	0.531 (3)
C02C	0.3017 (17)	0.1852 (14)	0.0611 (9)	0.105 (5)*	0.234 (3)
H02G	0.2904	0.2531	0.0922	0.158*	0.234 (3)
H02H	0.2404	0.1256	0.0697	0.158*	0.234 (3)
H02I	0.2782	0.1862	0.0102	0.158*	0.234 (3)
O01C	0.5292 (12)	0.2218 (9)	0.1318 (6)	0.114 (4)*	0.234 (3)
C01C	0.4361 (18)	0.1723 (14)	0.0770 (9)	0.105 (5)*	0.234 (3)
C03C	0.520 (3)	0.075 (2)	0.0452 (15)	0.207 (13)*	0.234 (3)
H03G	0.6172	0.0946	0.0697	0.311*	0.234 (3)
H03H	0.5138	0.0654	−0.0070	0.311*	0.234 (3)
H03I	0.4779	0.0079	0.0542	0.311*	0.234 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.02396 (3)	0.02515 (3)	0.03438 (3)	0.00362 (2)	0.00467 (2)	0.00605 (2)
Ir1′	0.03068 (3)	0.03418 (4)	0.03286 (3)	0.00177 (3)	0.00719 (3)	0.00033 (3)
O1	0.0266 (5)	0.0334 (6)	0.0379 (6)	0.0055 (5)	0.0094 (5)	0.0082 (5)
O2	0.0268 (5)	0.0354 (6)	0.0368 (6)	0.0062 (5)	0.0074 (5)	0.0091 (5)
O1′	0.0319 (6)	0.0367 (7)	0.0379 (7)	0.0000 (5)	0.0091 (5)	0.0001 (6)
O2′	0.0366 (6)	0.0360 (7)	0.0403 (7)	−0.0010 (6)	0.0076 (6)	0.0024 (6)
N1	0.0286 (7)	0.0312 (7)	0.0393 (8)	0.0035 (6)	0.0055 (6)	0.0110 (6)
N2	0.0282 (7)	0.0297 (7)	0.0414 (8)	0.0046 (6)	0.0084 (6)	0.0034 (6)
N1′	0.0304 (7)	0.0468 (9)	0.0379 (8)	−0.0028 (7)	0.0119 (6)	0.0043 (7)
N2′	0.0436 (9)	0.0342 (8)	0.0396 (9)	0.0032 (7)	0.0050 (7)	−0.0037 (7)
C1	0.0365 (9)	0.0324 (9)	0.0485 (10)	0.0025 (8)	0.0116 (8)	0.0060 (8)
C2	0.0503 (12)	0.0359 (11)	0.0676 (14)	−0.0027 (10)	0.0145 (11)	−0.0044 (11)
C3	0.0412 (11)	0.0448 (12)	0.0789 (16)	−0.0136 (10)	0.0116 (11)	−0.0070 (12)
C4	0.0345 (10)	0.0431 (11)	0.0689 (14)	−0.0035 (9)	0.0091 (10)	−0.0009 (11)
C5	0.0292 (8)	0.0335 (8)	0.0460 (10)	0.0056 (7)	0.0059 (7)	0.0109 (8)
C6	0.0285 (8)	0.0326 (8)	0.0434 (10)	0.0057 (7)	0.0051 (7)	0.0109 (7)
C7	0.0277 (8)	0.0467 (11)	0.0610 (12)	0.0038 (8)	0.0102 (8)	0.0142 (9)
C8	0.0386 (9)	0.0592 (12)	0.0690 (13)	0.0252 (8)	0.0217 (9)	0.0140 (11)
C9	0.0500 (11)	0.0436 (10)	0.0632 (13)	0.0184 (9)	0.0162 (10)	0.0060 (10)
C10	0.0352 (9)	0.0358 (9)	0.0415 (10)	0.0062 (8)	0.0069 (8)	0.0060 (8)
C11	0.0320 (8)	0.0292 (8)	0.0322 (8)	0.0057 (7)	0.0046 (7)	0.0105 (6)
C12	0.0313 (8)	0.0423 (10)	0.0407 (10)	0.0059 (8)	0.0083 (8)	−0.0014 (8)
C13	0.0379 (10)	0.0460 (11)	0.0475 (12)	0.0020 (9)	−0.0009 (9)	−0.0095 (10)
C14	0.0371 (10)	0.0396 (11)	0.0789 (16)	−0.0056 (9)	0.0076 (11)	−0.0078 (12)
C15	0.0481 (11)	0.0350 (10)	0.0648 (13)	−0.0097 (9)	0.0139 (10)	0.0059 (10)
C16	0.0323 (8)	0.0292 (9)	0.0466 (10)	−0.0012 (7)	0.0113 (8)	0.0000 (8)
C17	0.0413 (9)	0.0308 (8)	0.0457 (10)	0.0047 (8)	0.0150 (8)	0.0108 (8)
C18	0.0609 (13)	0.0347 (10)	0.0655 (13)	0.0041 (9)	0.0223 (10)	0.0156 (9)
C19	0.0686 (14)	0.0495 (11)	0.0550 (11)	0.0168 (10)	0.0196 (10)	0.0278 (9)
C20	0.0616 (13)	0.0487 (11)	0.0460 (11)	0.0096 (10)	0.0059 (10)	0.0153 (9)
C21	0.0449 (10)	0.0440 (10)	0.0410 (10)	0.0075 (9)	0.0038 (9)	0.0143 (8)

C22	0.0303 (8)	0.0315 (8)	0.0394 (9)	0.0094 (7)	0.0104 (7)	0.0108 (7)
C23	0.0234 (7)	0.0272 (8)	0.0320 (8)	−0.0003 (6)	0.0022 (6)	0.0062 (7)
C1′	0.0439 (10)	0.0466 (11)	0.0421 (10)	0.0011 (9)	0.0147 (8)	0.0089 (9)
C2′	0.0425 (10)	0.0593 (12)	0.0498 (11)	0.0047 (10)	0.0124 (9)	0.0193 (10)
C3′	0.0372 (10)	0.0781 (15)	0.0406 (10)	0.0004 (10)	0.0051 (9)	0.0214 (10)
C4′	0.0335 (9)	0.0543 (12)	0.0420 (10)	−0.0049 (9)	0.0064 (8)	0.0070 (9)
C5′	0.0289 (8)	0.0497 (11)	0.0372 (9)	−0.0063 (8)	0.0103 (7)	0.0005 (9)
C6′	0.0308 (8)	0.0475 (11)	0.0380 (9)	−0.0007 (8)	0.0125 (7)	0.0023 (8)
C7′	0.0363 (10)	0.0552 (13)	0.0474 (11)	−0.0050 (10)	0.0123 (9)	−0.0058 (10)
C8′	0.0598 (13)	0.0416 (12)	0.0568 (13)	−0.0038 (10)	0.0210 (10)	−0.0061 (10)
C9′	0.0795 (15)	0.0417 (12)	0.0597 (13)	0.0111 (11)	0.0240 (12)	0.0027 (11)
C10′	0.0526 (12)	0.0442 (11)	0.0482 (11)	0.0044 (10)	0.0152 (9)	0.0027 (10)
C11′	0.0351 (9)	0.0376 (10)	0.0388 (9)	0.0023 (8)	0.0113 (8)	−0.0011 (8)
C12′	0.0695 (15)	0.0490 (12)	0.0476 (13)	0.0110 (11)	0.0031 (12)	0.0061 (10)
C13′	0.094 (2)	0.0700 (15)	0.0492 (14)	0.0200 (14)	−0.0052 (14)	0.0205 (12)
C14′	0.0770 (16)	0.0614 (14)	0.0746 (17)	0.0242 (12)	−0.0166 (14)	0.0156 (13)
C15′	0.0551 (13)	0.0511 (13)	0.0734 (17)	0.0168 (11)	−0.0101 (13)	0.0006 (12)
C16′	0.0423 (11)	0.0379 (10)	0.0539 (13)	0.0052 (9)	0.0002 (10)	−0.0063 (10)
C17′	0.0343 (9)	0.0377 (10)	0.0598 (13)	0.0023 (8)	0.0049 (9)	−0.0088 (10)
C18′	0.0357 (11)	0.0551 (14)	0.0786 (17)	0.0020 (10)	0.0074 (11)	−0.0125 (13)
C19′	0.0437 (11)	0.0632 (15)	0.0770 (15)	−0.0098 (11)	0.0286 (10)	−0.0125 (13)
C20′	0.0553 (11)	0.0543 (14)	0.0604 (12)	−0.0110 (11)	0.0312 (9)	−0.0047 (11)
C21′	0.0459 (11)	0.0488 (12)	0.0498 (11)	−0.0011 (10)	0.0187 (9)	−0.0032 (10)
C22′	0.0390 (9)	0.0298 (9)	0.0420 (10)	−0.0012 (8)	0.0097 (8)	−0.0057 (8)
C23′	0.0289 (8)	0.0359 (9)	0.0284 (8)	0.0014 (7)	0.0029 (7)	0.0026 (7)
O101	0.1261 (18)	0.0697 (12)	0.130 (2)	0.0374 (12)	0.0192 (16)	0.0166 (13)
C101	0.0609 (18)	0.112 (2)	0.130 (3)	0.0122 (18)	0.0012 (19)	0.045 (2)
C102	0.0777 (17)	0.0599 (14)	0.0788 (18)	0.0229 (13)	0.0025 (15)	0.0196 (13)
C103	0.101 (2)	0.0619 (18)	0.121 (3)	0.0099 (18)	−0.002 (2)	0.0197 (18)
C01A	0.106 (3)	0.061 (3)	0.110 (3)	0.005 (3)	0.028 (3)	0.002 (3)
C02A	0.120 (4)	0.095 (4)	0.234 (6)	−0.007 (3)	0.085 (4)	0.015 (4)
C03A	0.120 (4)	0.095 (4)	0.234 (6)	−0.007 (3)	0.085 (4)	0.015 (4)
O01A	0.133 (3)	0.077 (2)	0.173 (4)	0.020 (2)	−0.004 (3)	0.032 (2)
C01B	0.106 (3)	0.061 (3)	0.110 (3)	0.005 (3)	0.028 (3)	0.002 (3)
C02B	0.120 (4)	0.095 (4)	0.234 (6)	−0.007 (3)	0.085 (4)	0.015 (4)
C03B	0.120 (4)	0.095 (4)	0.234 (6)	−0.007 (3)	0.085 (4)	0.015 (4)
O01B	0.133 (3)	0.077 (2)	0.173 (4)	0.020 (2)	−0.004 (3)	0.032 (2)

Geometric parameters (Å, º)

Ir1—C22	1.979 (2)	C4′—C5′	1.392 (3)
Ir1—C11	1.9824 (19)	C4′—H4′	0.9500
Ir1—N1	2.0308 (13)	C5′—C6′	1.449 (3)
Ir1—N2	2.0429 (14)	C6′—C11′	1.403 (3)
Ir1—O2	2.1911 (14)	C6′—C7′	1.419 (3)
Ir1—O1	2.1938 (13)	C7′—C8′	1.372 (4)
Ir1′—C22′	1.980 (2)	C7′—H7′	0.9500
Ir1′—C11′	1.9876 (19)	C8′—C9′	1.354 (3)

Ir1′—N1′	2.0191 (17)	C8′—H8′	0.9500
Ir1′—N2′	2.0303 (18)	C9′—C10′	1.406 (3)
Ir1′—O1′	2.1931 (13)	C9′—H9′	0.9500
Ir1′—O2′	2.1969 (15)	C10′—C11′	1.399 (3)
O1—C23^{i}	1.238 (2)	C10′—H10′	0.9500
O2—C23	1.265 (2)	C12′—C13′	1.379 (4)
O1′—C23′^{ii}	1.254 (2)	C12′—H12′	0.9500
O2′—C23′	1.253 (2)	C13′—C14′	1.376 (5)
N1—C1	1.347 (2)	C13′—H13′	0.9500
N1—C5	1.362 (3)	C14′—C15′	1.342 (5)
N2—C12	1.344 (2)	C14′—H14′	0.9500
N2—C16	1.346 (3)	C15′—C16′	1.397 (4)
N1′—C1′	1.350 (3)	C15′—H15′	0.9500
N1′—C5′	1.374 (2)	C16′—C17′	1.447 (4)
N2′—C12′	1.355 (3)	C17′—C22′	1.409 (3)
N2′—C16′	1.356 (3)	C17′—C18′	1.419 (3)
C1—C2	1.364 (3)	C18′—C19′	1.364 (4)
C1—H1	0.9500	C18′—H18′	0.9500
C2—C3	1.365 (4)	C19′—C20′	1.376 (4)
C2—H2	0.9500	C19′—H19′	0.9500
C3—C4	1.379 (3)	C20′—C21′	1.400 (3)
C3—H3	0.9500	C20′—H20′	0.9500
C4—C5	1.383 (3)	C21′—C22′	1.403 (3)
C4—H4	0.9500	C21′—H21′	0.9500
C5—C6	1.460 (3)	C23′—O1′^{ii}	1.254 (2)
C6—C7	1.394 (3)	C23′—C23′^{ii}	1.550 (4)
C6—C11	1.419 (2)	O101—C102	1.227 (4)
C7—C8	1.367 (3)	C101—C102	1.426 (5)
C7—H7	0.9500	C101—H10A	0.9800
C8—C9	1.390 (3)	C101—H10B	0.9800
C8—H8	0.9500	C101—H10C	0.9800
C9—C10	1.378 (3)	C102—C103	1.464 (4)
C9—H9	0.9500	C103—H10D	0.9800
C10—C11	1.407 (3)	C103—H10E	0.9800
C10—H10	0.9500	C103—H10F	0.9800
C12—C13	1.374 (3)	C01A—O01A	1.219 (5)
C12—H12	0.9500	C01A—C03A	1.481 (6)
C13—C14	1.370 (4)	C01A—C02A	1.483 (6)
C13—H13	0.9500	C02A—H02A	0.9800
C14—C15	1.377 (3)	C02A—H02B	0.9800
C14—H14	0.9500	C02A—H02C	0.9800
C15—C16	1.396 (3)	C03A—H03A	0.9800
C15—H15	0.9500	C03A—H03B	0.9800
C16—C17	1.461 (3)	C03A—H03C	0.9800
C17—C18	1.397 (3)	C01B—O01B	1.207 (4)
C17—C22	1.403 (3)	C01B—C03B	1.475 (5)
C18—C19	1.371 (3)	C01B—C02B	1.479 (5)
C18—H18	0.9500	C02B—H02D	0.9800

C19—C20	1.381 (3)	C02B—H02E	0.9800
C19—H19	0.9500	C02B—H02F	0.9800
C20—C21	1.394 (4)	C03B—H03D	0.9800
C20—H20	0.9500	C03B—H03E	0.9800
C21—C22	1.399 (3)	C03B—H03F	0.9800
C21—H21	0.9500	C02C—C01C	1.37 (2)
C23—O1^{i}	1.238 (2)	C02C—H02G	0.9800
C23—C23^{i}	1.545 (4)	C02C—H02H	0.9800
C1′—C2′	1.383 (3)	C02C—H02I	0.9800
C1′—H1′	0.9500	O01C—C01C	1.268 (18)
C2′—C3′	1.366 (3)	C01C—C03C	1.67 (3)
C2′—H2′	0.9500	C03C—H03G	0.9800
C3′—C4′	1.378 (4)	C03C—H03H	0.9800
C3′—H3′	0.9500	C03C—H03I	0.9800

C22—Ir1—C11	89.83 (8)	C2′—C3′—H3′	119.8
C22—Ir1—N1	95.20 (7)	C4′—C3′—H3′	119.8
C11—Ir1—N1	80.72 (7)	C3′—C4′—C5′	120.03 (19)
C22—Ir1—N2	80.59 (7)	C3′—C4′—H4′	120.0
C11—Ir1—N2	99.37 (7)	C5′—C4′—H4′	120.0
N1—Ir1—N2	175.79 (7)	N1′—C5′—C4′	119.6 (2)
C22—Ir1—O2	173.61 (6)	N1′—C5′—C6′	112.81 (17)
C11—Ir1—O2	96.13 (7)	C4′—C5′—C6′	127.63 (18)
N1—Ir1—O2	88.05 (6)	C11′—C6′—C7′	120.3 (2)
N2—Ir1—O2	96.11 (6)	C11′—C6′—C5′	116.10 (17)
C22—Ir1—O1	98.03 (7)	C7′—C6′—C5′	123.55 (19)
C11—Ir1—O1	171.29 (7)	C8′—C7′—C6′	120.2 (2)
N1—Ir1—O1	94.75 (5)	C8′—C7′—H7′	119.9
N2—Ir1—O1	85.70 (5)	C6′—C7′—H7′	119.9
O2—Ir1—O1	76.18 (5)	C9′—C8′—C7′	119.6 (2)
C22′—Ir1′—C11′	89.48 (8)	C9′—C8′—H8′	120.2
C22′—Ir1′—N1′	96.51 (8)	C7′—C8′—H8′	120.2
C11′—Ir1′—N1′	80.88 (8)	C8′—C9′—C10′	122.2 (3)
C22′—Ir1′—N2′	80.65 (8)	C8′—C9′—H9′	118.9
C11′—Ir1′—N2′	94.79 (8)	C10′—C9′—H9′	118.9
N1′—Ir1′—N2′	174.88 (7)	C11′—C10′—C9′	119.5 (2)
C22′—Ir1′—O1′	96.80 (7)	C11′—C10′—H10′	120.2
C11′—Ir1′—O1′	172.17 (7)	C9′—C10′—H10′	120.2
N1′—Ir1′—O1′	93.72 (6)	C10′—C11′—C6′	118.21 (18)
N2′—Ir1′—O1′	90.86 (6)	C10′—C11′—Ir1′	127.65 (15)
C22′—Ir1′—O2′	172.30 (6)	C6′—C11′—Ir1′	114.14 (16)
C11′—Ir1′—O2′	97.62 (7)	N2′—C12′—C13′	121.3 (3)
N1′—Ir1′—O2′	87.60 (6)	N2′—C12′—H12′	119.3
N2′—Ir1′—O2′	95.72 (7)	C13′—C12′—H12′	119.3
O1′—Ir1′—O2′	76.38 (5)	C14′—C13′—C12′	118.2 (3)
C23^{i}—O1—Ir1	113.75 (12)	C14′—C13′—H13′	120.9
C23—O2—Ir1	113.94 (12)	C12′—C13′—H13′	120.9
C23′^{ii}—O1′—Ir1′	114.11 (11)	C15′—C14′—C13′	120.9 (3)

C23′—O2′—Ir1′	114.06 (12)	C15′—C14′—H14′	119.5
C1—N1—C5	119.93 (15)	C13′—C14′—H14′	119.5
C1—N1—Ir1	124.16 (13)	C14′—C15′—C16′	120.1 (3)
C5—N1—Ir1	115.87 (12)	C14′—C15′—H15′	120.0
C12—N2—C16	119.68 (16)	C16′—C15′—H15′	120.0
C12—N2—Ir1	124.68 (15)	N2′—C16′—C15′	119.3 (2)
C16—N2—Ir1	115.34 (12)	N2′—C16′—C17′	113.7 (2)
C1′—N1′—C5′	119.14 (18)	C15′—C16′—C17′	127.0 (2)
C1′—N1′—Ir1′	124.78 (12)	C22′—C17′—C18′	120.4 (2)
C5′—N1′—Ir1′	116.06 (15)	C22′—C17′—C16′	115.4 (2)
C12′—N2′—C16′	120.0 (2)	C18′—C17′—C16′	124.2 (2)
C12′—N2′—Ir1′	124.05 (16)	C19′—C18′—C17′	119.9 (2)
C16′—N2′—Ir1′	115.86 (16)	C19′—C18′—H18′	120.0
N1—C1—C2	122.2 (2)	C17′—C18′—H18′	120.0
N1—C1—H1	118.9	C18′—C19′—C20′	120.8 (2)
C2—C1—H1	118.9	C18′—C19′—H19′	119.6
C1—C2—C3	118.6 (2)	C20′—C19′—H19′	119.6
C1—C2—H2	120.7	C19′—C20′—C21′	120.2 (3)
C3—C2—H2	120.7	C19′—C20′—H20′	119.9
C2—C3—C4	120.1 (2)	C21′—C20′—H20′	119.9
C2—C3—H3	120.0	C20′—C21′—C22′	120.9 (2)
C4—C3—H3	120.0	C20′—C21′—H21′	119.5
C3—C4—C5	119.9 (2)	C22′—C21′—H21′	119.5
C3—C4—H4	120.1	C21′—C22′—C17′	117.6 (2)
C5—C4—H4	120.1	C21′—C22′—Ir1′	127.87 (16)
N1—C5—C4	119.25 (18)	C17′—C22′—Ir1′	114.45 (17)
N1—C5—C6	113.85 (15)	O2′—C23′—O1′^{ii}	124.65 (17)
C4—C5—C6	126.84 (19)	O2′—C23′—C23′^{ii}	117.6 (2)
C7—C6—C11	121.19 (17)	O1′^{ii}—C23′—C23′^{ii}	117.7 (2)
C7—C6—C5	124.29 (16)	C102—C101—H10A	109.5
C11—C6—C5	114.47 (17)	C102—C101—H10B	109.5
C8—C7—C6	120.62 (18)	H10A—C101—H10B	109.5
C8—C7—H7	119.7	C102—C101—H10C	109.5
C6—C7—H7	119.7	H10A—C101—H10C	109.5
C7—C8—C9	119.3 (2)	H10B—C101—H10C	109.5
C7—C8—H8	120.3	O101—C102—C101	122.7 (3)
C9—C8—H8	120.3	O101—C102—C103	120.3 (3)
C10—C9—C8	121.0 (2)	C101—C102—C103	117.1 (3)
C10—C9—H9	119.5	C102—C103—H10D	109.5
C8—C9—H9	119.5	C102—C103—H10E	109.5
C9—C10—C11	121.36 (17)	H10D—C103—H10E	109.5
C9—C10—H10	119.3	C102—C103—H10F	109.5
C11—C10—H10	119.3	H10D—C103—H10F	109.5
C10—C11—C6	116.48 (17)	H10E—C103—H10F	109.5
C10—C11—Ir1	128.71 (13)	O01A—C01A—C03A	121.5 (7)
C6—C11—Ir1	114.76 (13)	O01A—C01A—C02A	119.6 (6)
N2—C12—C13	122.5 (2)	C03A—C01A—C02A	116.3 (6)
N2—C12—H12	118.8	C01A—C02A—H02A	109.5

C13—C12—H12	118.8	C01A—C02A—H02B	109.5
C14—C13—C12	118.9 (2)	H02A—C02A—H02B	109.5
C14—C13—H13	120.5	C01A—C02A—H02C	109.5
C12—C13—H13	120.5	H02A—C02A—H02C	109.5
C13—C14—C15	118.8 (2)	H02B—C02A—H02C	109.5
C13—C14—H14	120.6	C01A—C03A—H03A	109.5
C15—C14—H14	120.6	C01A—C03A—H03B	109.5
C14—C15—C16	120.5 (2)	H03A—C03A—H03B	109.5
C14—C15—H15	119.7	C01A—C03A—H03C	109.5
C16—C15—H15	119.7	H03A—C03A—H03C	109.5
N2—C16—C15	119.52 (19)	H03B—C03A—H03C	109.5
N2—C16—C17	114.02 (16)	O01B—C01B—C03B	122.9 (5)
C15—C16—C17	126.4 (2)	O01B—C01B—C02B	121.7 (4)
C18—C17—C22	121.21 (18)	C03B—C01B—C02B	114.9 (4)
C18—C17—C16	123.91 (18)	C01B—C02B—H02D	109.5
C22—C17—C16	114.87 (19)	C01B—C02B—H02E	109.5
C19—C18—C17	120.4 (2)	H02D—C02B—H02E	109.5
C19—C18—H18	119.8	C01B—C02B—H02F	109.5
C17—C18—H18	119.8	H02D—C02B—H02F	109.5
C18—C19—C20	119.5 (2)	H02E—C02B—H02F	109.5
C18—C19—H19	120.3	C01B—C03B—H03D	109.5
C20—C19—H19	120.3	C01B—C03B—H03E	109.5
C19—C20—C21	120.7 (2)	H03D—C03B—H03E	109.5
C19—C20—H20	119.7	C01B—C03B—H03F	109.5
C21—C20—H20	119.7	H03D—C03B—H03F	109.5
C20—C21—C22	120.94 (19)	H03E—C03B—H03F	109.5
C20—C21—H21	119.5	C01C—C02C—H02G	109.5
C22—C21—H21	119.5	C01C—C02C—H02H	109.5
C21—C22—C17	117.2 (2)	H02G—C02C—H02H	109.5
C21—C22—Ir1	127.91 (15)	C01C—C02C—H02I	109.5
C17—C22—Ir1	114.84 (13)	H02G—C02C—H02I	109.5
O1^{i}—C23—O2	124.74 (18)	H02H—C02C—H02I	109.5
O1^{i}—C23—C23^{i}	118.6 (2)	O01C—C01C—C02C	128.7 (17)
O2—C23—C23^{i}	116.7 (2)	O01C—C01C—C03C	96.8 (15)
N1′—C1′—C2′	122.61 (19)	C02C—C01C—C03C	133.0 (15)
N1′—C1′—H1′	118.7	C01C—C03C—H03G	109.5
C2′—C1′—H1′	118.7	C01C—C03C—H03H	109.5
C3′—C2′—C1′	118.3 (2)	H03G—C03C—H03H	109.5
C3′—C2′—H2′	120.8	C01C—C03C—H03I	109.5
C1′—C2′—H2′	120.8	H03G—C03C—H03I	109.5
C2′—C3′—C4′	120.4 (2)	H03H—C03C—H03I	109.5

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z$.